

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	4	("20030060459" "20030216434" "6011052" "6706712").PN.	US-PGPUB; USPAT	OR	ON	2006/12/13 13:24
L2	4	("20040110736" "20040235836" "20040235835" "20050043392").PN.	US-PGPUB; USPAT	OR	ON	2006/12/13 13:43
L3	1	("20030171218").PN.	US-PGPUB; USPAT.	OR	ON	2006/12/13 15:31
L4	885	548/518.ccls.	US-PGPUB; USPAT	OR	ON	2006/12/13 15:31

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive
NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced
NEWS 5 AUG 30 CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6 SEP 11 CA/CAplus enhanced with more pre-1907 records
NEWS 7 SEP 21 CA/CAplus fields enhanced with simultaneous left and right
truncation
NEWS 8 SEP 25 CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new
classification scheme
NEWS 12 OCT 19 LOGOFF HOLD duration extended to 120 minutes
NEWS 13 OCT 19 E-mail format enhanced
NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available
NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in
multiple databases
NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN
has been enhanced and reloaded
NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field
NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality
NEWS 19 NOV 10 CA/CAplus F-Term thesaurus enhanced
NEWS 20 NOV 10 STN Express with Discover! free maintenance release Version
8.01c now available
NEWS 21 NOV 13 CA/CAplus pre-1967 chemical substance index entries enhanced
with preparation role
NEWS 22 NOV 20 CAS Registry Number crossover limit increased to 300,000 in
additional databases
NEWS 23 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased
to 50,000
NEWS 24 NOV 20 CA/CAplus patent kind codes will be updated
NEWS 25 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 26 DEC 11 CAS REGISTRY chemical nomenclature enhanced

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:26:24 ON 13 DEC 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:26:36 ON 13 DEC 2006

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STRUCTURE FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

DICTIONARY FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

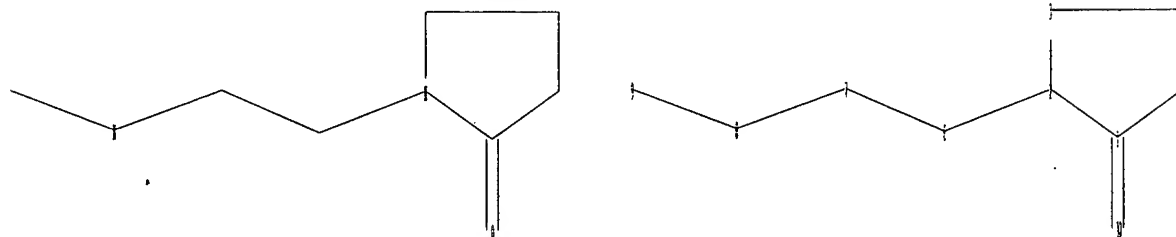
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 1.str



chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :

10776586.trn

Page 3

1-10 2-6 6-7 7-8 8-9

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9

exact bonds :

6-7

Match level :

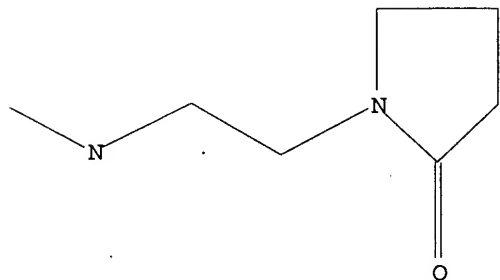
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 10:26:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2466 TO ITERATE

81.1% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

50 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 46342 TO 52298

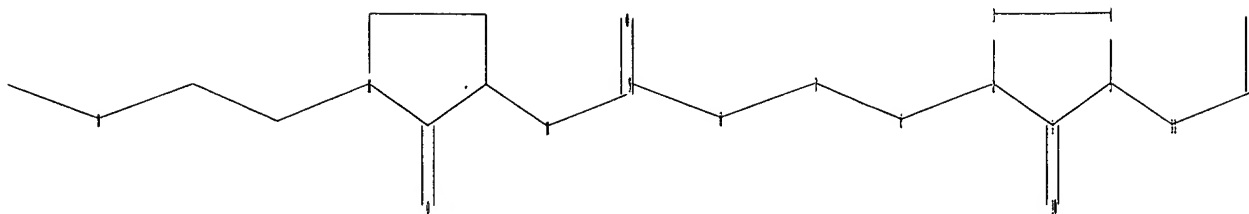
PROJECTED ANSWERS: 11745 TO 14837

L2 50 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 2.str

10776586.trn



chain nodes :

6 7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5

chain bonds :

1-10 2-6 5-11 6-7 7-8 8-9 11-12 12-13

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 5-11 7-8 8-9 11-12 12-13

exact bonds :

6-7

Match level :

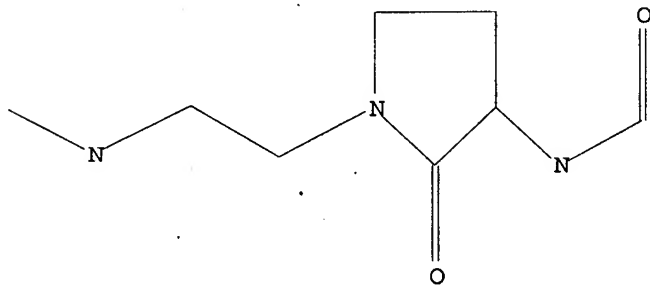
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> 13

SAMPLE SEARCH INITIATED 10:27:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 79 TO ITERATE

100.0% PROCESSED 79 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

10776586.trn

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 1047 TO 2113
 PROJECTED ANSWERS: 592 TO 1448

L4 50 SEA SSS SAM L3

=> 13 full
 FULL SEARCH INITIATED 10:27:41 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 1291 TO ITERATE

100.0% PROCESSED 1291 ITERATIONS 874 ANSWERS
 SEARCH TIME: 00.00.01

L5 874 SEA SSS FUL L3

=> file medline caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	167.38	167.59

FILE 'MEDLINE' ENTERED AT 10:27:48 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:27:48 ON 13 DEC 2006
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 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

=> 15
 L6 300 L5

=> dup rem 16
 PROCESSING COMPLETED FOR L6
 L7 284 DUP REM L6 (16 DUPLICATES REMOVED)

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	18.33	185.92

FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006
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STRUCTURE FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1
 DICTIONARY FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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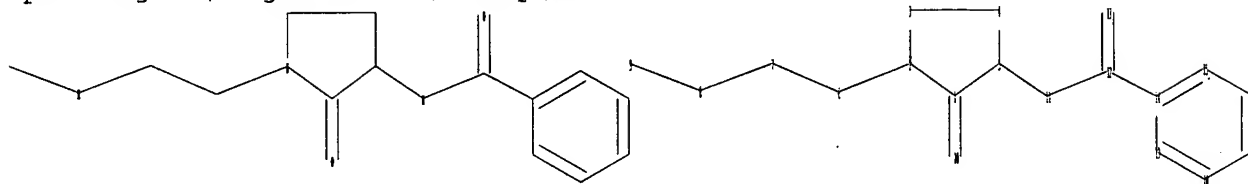
REGISTRY includes numerically searchable data for experimental and

predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 3.str



chain nodes :

6 7 8 9 10 11 12 13

ring nodes :

1 2 3 4 5 14 15 16 17 18 19

chain bonds :

1-10 2-6 5-11 6-7 7-8 8-9 11-12 12-13 12-14

ring bonds :

1-2 1-5 2-3 3-4 4-5 14-15 14-19 15-16 16-17 17-18 18-19

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 5-11 7-8 8-9 11-12 12-13

exact bonds :

6-7 12-14

normalized bonds :

14-15 14-19 15-16 16-17 17-18 18-19

Match level :

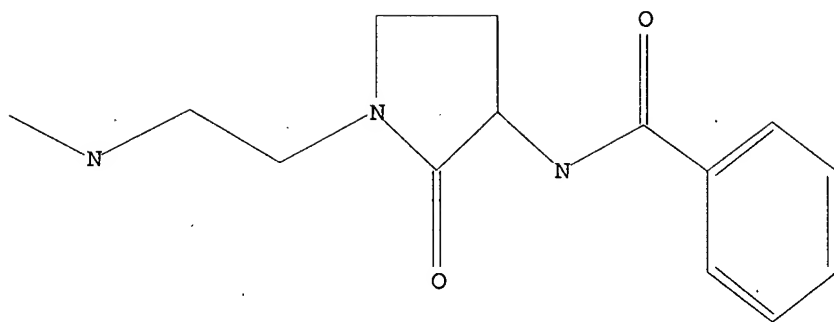
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom
19:Atom

L8 STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

=> l8

SAMPLE SEARCH INITIATED 10:28:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 146 TO 694
PROJECTED ANSWERS: 1 TO 80

L9 1 SEA SSS SAM L8

=> l8 full

FULL SEARCH INITIATED 10:28:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 394 TO ITERATE

100.0% PROCESSED 394 ITERATIONS 23 ANSWERS
SEARCH TIME: 00.00.01

L10 23 SEA SSS FUL L8

=> file medline caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	166.94	352.86

FILE 'MEDLINE' ENTERED AT 10:28:52 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:28:52 ON 13 DEC 2006
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=> l10

L11 8 L10

=> dup rem l11

PROCESSING COMPLETED FOR L11
L12 8 DUP REM L11 (0 DUPLICATES REMOVED)

10776586.trn

Page 8

=> d ibib abs hitstr 1-8

10776586.trn

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:701971 CAPLUS

DOCUMENT NUMBER: 141:225303

TITLE: Preparation of N-[(benzylaminomethyl)alkyl]-2-(acylamino)pyrrolidinones as modulators of chemokine receptor activity

INVENTOR(S): Carter, Percy; Voas, Matthew E.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 140 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004071449	A2	20040826	WO 2004-US4151	20040211
WO 2004071449	A3	20050106		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW, BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, NG, SN, TD, TG

US 2004186143 A1 20040923 US 2004-776586 20040211
 PRIORITY APPLN. INFO.: US 2003-446976P P 20030212

OTHER SOURCE(S): MARPAT 141:225303
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Lactams I [A = (CHR14)n; E = CH2CH2, CH:CH; Q = O, S; R1, R2 = (un)substituted aryl or heteroaryl containing N, O, or S atoms; R3, R6, R7, R8, R9, R10, R11, R12 = H, (un)substituted hydroxyalkyl, mercaptoalkyl, alkoxyalkyl, sulfinylalkyl, sulfonylalkyl, etc.; R13, R14 = H, (un)substituted alkyl; R16, R17 = H, (un)substituted alkyl, cycloalkyl; X = NR17, CHR16NR17; Z = bond, (un)substituted aminocarbonyl, carbonylamino, aminothiocarbonyl, aminosulfonyl, aminosulfonylamino, etc.; m, q = 0-1; n = 0-3; p = 0-1], particularly the N-[(benzylaminomethyl)alkyl]-2-(acylamino)pyrrolidinones II [R20 = 3-(F3C)C6H4, 3-(F3C)C6H4NH, 2-(BocNH)-5-(F3C)C6H3, 2-H2N-5-(F3C)C6H3, 3-H2N-5-(F3C)C6H3] and III, are prepared as chemokine receptor modulators for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer and diseases related to organ transplantation. (S,S)-CbzNHC(CH2CH(NHBoc)CH(OH)C.tpbond.CMe is deprotected with trifluoroacetic acid and acylated with Boc-methionine with BOP;

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

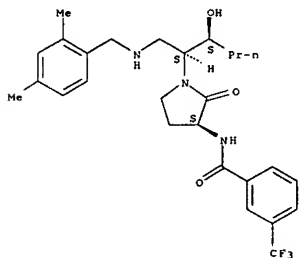
rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer)

RN 747149-73-1 CAPLUS

CN Benzamide,

N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

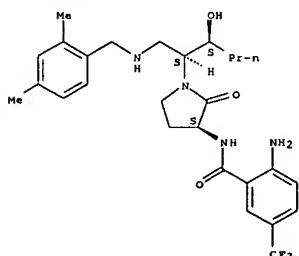
Absolute stereochemistry.



RN 747149-88-8 CAPLUS

CN Benzamide, 2-amino-N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 747149-95-7 CAPLUS

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L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

methylation of the thiomethyl group with Me iodide, cyclization with sodium hydride, hydrogenolysis of the Cbz protecting group and redn. of the alkyne, reductive amination of the free amine with 2,4-dimethylbenzaldehyde and reprecipitation of the secondary amino group with a Cbz moiety, Boc deprotection, BOP-mediated acylation with 3-trifluoromethylbenzoic acid, and hydrogenolysis of the Cbz protecting group yields II [R20 = 3-(F3C)C6H4]. Comps. of the invention inhibit MCP-1 binding to human peripheral blood mononuclear cells by 50% at concn. of <20µM (no data).

IT 747149-84-4P

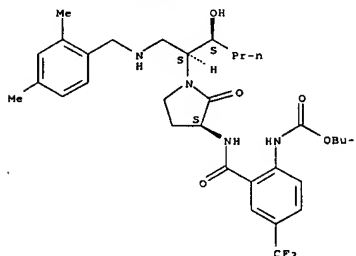
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine

receptor modulating agents for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer)

RN 747149-84-4 CAPLUS

CN Carbamic acid, [2-[[[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 747149-73-1P 747149-88-8P 747149-95-7P

747150-00-1P

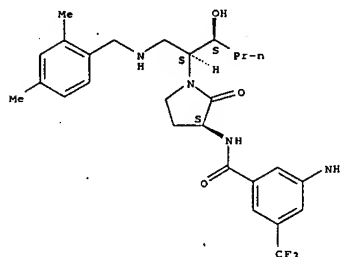
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine

receptor modulating agents for the treatment of diseases such as

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CN Benzamide, 3-amino-N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

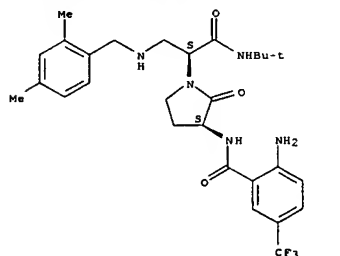
Absolute stereochemistry.



RN 747150-00-1 CAPLUS

CN 1-Pyrrolidineacetamide, 3-[[[2-amino-5-(trifluoromethyl)benzoyl]amino]-N-(1,1-dimethylethyl)-u-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxo-, (uS,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

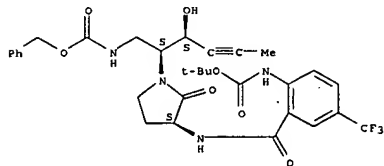


IT 747150-20-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 receptor modulating agents for the treatment of diseases such as
 rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma,
 restenosis, and cancer)
 RN 747150-20-5 CAPLUS
 CN Carbamic acid,
 [(2S,3S)-2-[(3S)-3-[[2-[[[1,1-dimethylethoxy]carbonyl]amino
]-5-(trifluoromethyl)benzoyl]amino]-2-oxo-1-pyrrolidinyl]-3-hydroxy-4-
 hexynyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

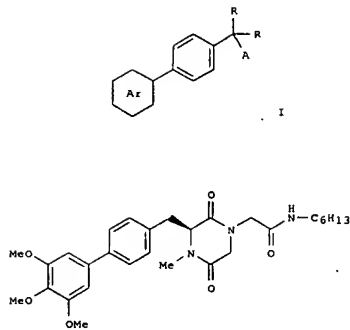


L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2002:695961 CAPLUS
 DOCUMENT NUMBER: 137:216961
 TITLE: Preparation of bisaryl derivatives having FSH
 receptor
 modulatory activity
 INVENTOR(S): Guo, Tao; He, Koc-Kan; McDonald, Edward; Dolle,
 Roland
 Ellwood; Saionz, Kurt W.; Kultgen, Steven G.; Liu,
 Ruiyan; Dong, Guizhen; Geng, Peng; Adang, Anton
 Egbert
 Peter: Van Straten, Nicole Corine Renee
 PATENT ASSIGNEE(S): Pharmacoceia, Inc., USA
 SOURCE: PCT Int. Appl., 167 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002070493	A1	20020912	WO 2002-US3777	20020118
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG			
CA 2434184	AA	20020912	CA 2002-2434184	20020118
EP 1351941	A1	20031015	EP 2002-717403	20020118
EP 1351941	B1	20040929		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
AT 277913	E	20041015	AT 2002-717403	20020118
JP 2005505496	T2	20050224	JP 2002-569813	20020118
US 2004152703	A1	20040805	US 2003-623640	20030721
US 6900213	B2	20050531		
PRIORITY APPLN. INFO.:			EP 2001-200194	A 20010119
			WO 2002-US3777	W 20020118

OTHER SOURCE(S): MARPAT 137:216961
 GI

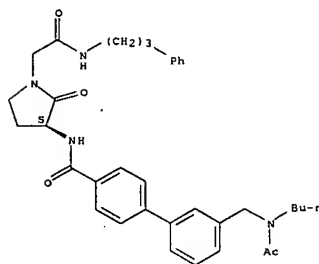
L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title compds. I [R,R = H/H, O, H/Me, H/OH, H/CN; A = pyridazinedione, etc.].
 Ar = (un)substituted phenyl were prepared. For example, a
 photolabile-supported 1-hexylamine derivative was acylated with
 (3S)-1-carboxymethyl-3-(4-iodobenzyl)-4-methyl-2,5-dioxopiperazine
 (preparation
 given) followed by coupling of the resulting aryl iodide with
 3,4,5-trimethoxybenzeneboronic acid (DME/EtOH, Pd2(dba)3, Ph3As, CsF).
 The resulting resin was irradiated at 365 nm at 50° (MeOH/TFA) to
 yield II. II had EC50 < 10 µM for the FSH receptor. I are useful in
 the treatment for the control of fertility, for contraception or for
 treatment of hormone-dependent disorders.
 IT 457614-55-OP
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
 (FSH receptor modulator; preparation of pyridazinedione-substituted
 bisaryl
 deriva. having FSH receptor modulatory activity)
 RN 457614-55-0 CAPLUS
 CN 1-Pyrrolidineacetamide,
 3-[[[3'-[(acetylbutylamino)methyl][1,1'-biphenyl]-
 4-yl]carbonyl]amino]-2-oxo-N-(3-phenylpropyl)-, (3S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

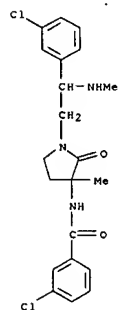
L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:824216 CAPLUS
 DOCUMENT NUMBER: 134:4857
 TITLE: Preparation of 3-acylamino-3-methylpyrrolidin-2-ones and analogs as metabotropic glutamate receptor antagonists
 INVENTOR(S): Clark, Barry Peter; Cwi, Cynthia Lynn; Harris, John Richard; Kingston, Ann Elizabeth; Scott, William Leonard
 PATENT ASSIGNEE(S): Eli Lilly and Company, USA
 SOURCE: PCT Int. Appl., 103 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000069816	A1	20001123	WO 2000-US8223	20000517
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1183238	A1	20020306	EP 2000-930094	20000517
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
PRIORITY APPLN. INFO.:			US 1999-134410P	P 19990517
			WO 2000-US8223	W 20000517

OTHER SOURCE(S): MARPAT 134:4857
 G1

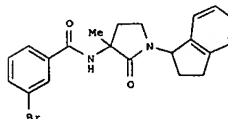
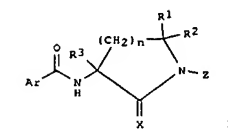
L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 (prepn. of 3-acylamino-3-methylpyrrolidin-2-ones and analogs by conventional and soln. phase combinatorial methods as metabotropic glutamate receptor antagonists)
 RN* 308817-13-2 CAPLUS
 CW Benzamide, 3-chloro-N-[1-(2-(3-chlorophenyl)-2-(methylamino)ethyl)-3-methyl-2-oxo-3-pyrrolidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The title compds. (I) (wherein n = 0-2; X = O, S, NH, or NOH; R1 and R2 = independently H, CN, CO2R, CONHR, alkyl, or tetrazole; or R1 and R2 together = :O; R = H or alkyl; R3 = (cyclo)alkyl, alkenyl, CH2OH, alkoxyethyl, or CO2H; Ar = (un)substituted (hetero)aromatic group; Z = (un)substituted indenyl, indenyl, phenylalkyl, phenylcyclopropyl, or CH2Bhet; B = CHR, CR2, alkyl, CO, CHO, CH2O, CH=CH, CH2CO, CH2S, CH2S(O), CH2SO2, CHCO2R, or CHNR2; Het = heterocycle) were prepared by conventional and solution phase combinatorial methods for the treatment or prevention of a physiologic disorder associated with an excess of stimulation of the human Group I metabotropic glutamate receptors, especially those designated as mGluR5. Examples include syntheses and phys. data for approx. 140 compds., description of bioassays with data summaries, and 8 pharmaceutical formulations employing I. Thus, (R,R)-II was prepared by reductive amination of N-(3-bromobenzoyl)-N-(2-oxoethyl)alanine (preparation given) with R-(-)-1-aminoindane in the presence of NaBH4 in MeOH followed by spontaneous cyclization to the lactam. When mGluR5 expressing cell lines were used, representative compds. of the invention generated IC50 values of < 30 μM in a phosphoinositide assay and resulted in 2-70% inhibition at concns. of 30 μM in a calcium flux assay. I are useful in the treatment of neurodegenerative conditions and pain (no data).
 IT 308817-13-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

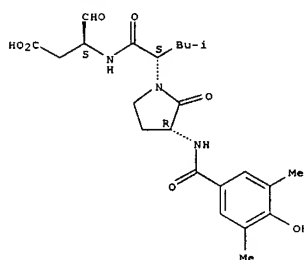
L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:613942 CAPLUS
 DOCUMENT NUMBER: 131:243593
 TITLE: Preparation of peptides as inhibitors of caspases
 INVENTOR(S): Wannamaker, Marion W.; Bemis, Guy W.; Charifson, Paul S.; Lauffer, David J.; Mullican, Michael D.; Murcko, Mark A.; Wilson, Keith P.; Janetka, James W.; Davies, Robert J.; Grillot, Anne-Laure; Shi, Zhan; Forster, Cornelia J.
 PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
 SOURCE: PCT Int. Appl., 297 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9947545	A2	19990923	WO 1999-US5919	19990319
WO 9947545	A3	19991125		
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2324226	A1	19990923	CA 1999-2324226	19990319
AU 9930986	A1	19991011	AU 1999-30986	19990319
AU 769033	B2	20040115		
BR 9909660	A	20001121	BR 1999-9660	19990319
EP 1064298	A2	20010103	EP 1999-912662	19990319
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
HU 200103575	A2	20020228	HU 2001-3575	19990319
JP 2002506878	T2	20020305	JP 2000-536738	19990319
TR 200103406	T2	20020621	TR 2001-200103406	19990319
NZ 506963	A	20031031	NZ 1999-506963	19990319
NZ 528282	A	20050527	NZ 1999-528282	19990319
TW 243828	B1	20051121	TW 1999-88104386	19990319
RU 2274642	C2	20060420	RU 2000-126298	19990319
ZA 2000004652	A	20020205	ZA 2000-4652	20000905
NO 2000004546	A	20001109	NO 2000-4546	20000912
US 6531474	B1	20030311	US 2000-665503	20000919
BG 104863	A	20010430	BG 2000-104863	20001016
US 2003232986	A1	20031218	US 2002-314103	20021206
AU 2003255217	A1	20031113	AU 2003-255217	20031022
JP 2006206600	A2	20060810	JP 2006-75461	20060317
PRIORITY APPLN. INFO.:			US 1998-78770P	A1 19980319
			AU 1999-30986	A3 19990319
			JP 2000-536738	A3 19990319
			WO 1999-US5919	W 19990319
			US 2000-665503	A3 20000919

L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 OTHER SOURCE(S): MARPAT 131:243593
 AB Peptides R1NR2XCONR4CR52CONHY [Y = CH(CHO)CH2(CH2)mCOR7, (m = 0 or 1 and R7 = OH or ester, NHOH) or cyclic lactol derivative when R7 is OH; X = CR32 or NR3 (R3 = H, an amino acid side chain, alkyl, cycloalkyl, aryl, etc.); R1 = H, R8, COR8, COCOR8, SO2R8, SOR8, CO2R8, CONHR8, SO2NHR8, SONHR8, COCONHR8, COCH:CHNR8, etc. (R8 = alkyl, cycloalkyl, aryl, etc.); R2 = H or R2 and R3 may form a ring; R4 = H and R5 = H, amino acid side chain, R8, etc. or R4 and R5 may form a ring] were prepared as inhibitors of caspases.
 Thus, p-AcNHCH6H4CO-L-Val-L-Pro-NHCH(CHO)CH2CO2H-(S) was prepared by the solid-phase method and showed $k_i < 10$ nm for inhibition of interleukin-1 β converting enzyme (ICE, caspase-1).
 IT 244132-96-5P 244132-97-6P 244132-99-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of peptides as inhibitors of caspases)
 RN 244132-96-5 CAPLUS
 CN Butanoic acid, 3-[[[(2S)-2-[[[(3R)-3-[[4-(4-hydroxy-3,5-dimethylbenzoyl)amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

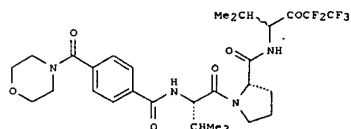
Absolute stereochemistry.



RN 244132-97-6 CAPLUS
 CN Butanoic acid, 3-[[[(2S)-2-[[[(3R)-3-[[1H-benzotriazol-5-ylcarbonyl]amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

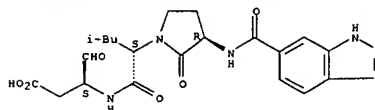
Absolute stereochemistry.

L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:430286 CAPLUS
 DOCUMENT NUMBER: 129:41393
 TITLE: Inhibition of Human Neutrophil Elastase. 4. Design, Synthesis, X-ray Crystallographic Analysis, and Structure-Activity Relationships for a Series of P2-Modified, Orally Active Peptidyl Pentafluoroethyl Ketones
 AUTHOR(S): Cregge, Robert J.; Durham, Sherrie L.; Farr, Robert A.; Gallion, Steven L.; Hare, C. Michelle; Hoffman, Robert V.; Janusz, Michael J.; Kim, Hwa-Ok; Koehl, Jack R.; Mehdi, Shujaath; Metz, William A.; Peet, Merton P.; Pelton, John T.; Schreuder, Herman A.; Sunder, Shyam; Tardif, Chantal
 CORPORATE SOURCE: Hoechst Marion Roussel Inc., Cincinnati, OH, 45215, USA
 SOURCE: Journal of Medicinal Chemistry (1998), 41(14), 2461-2480
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



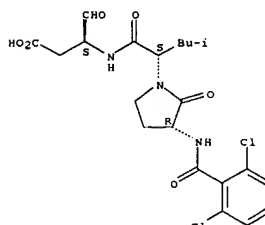
AB A series of P2-modified, orally active peptidic inhibitors of human neutrophil elastase (HNE) are reported. These pentafluoroethyl ketone-based inhibitors were designed using pentafluoroethyl ketone I (MDL 101,146) as a model. Rational structural modifications were made at the P3, P2, and activating group (AG) portions of I based on structure-activity relationships (SAR) developed from in vitro (measured K_i) data and information provided by modeling studies that docked inhibitor I into the active site of HNE. The modeling-based design was corroborated with X-ray crystallog. anal. of the complex between I and porcine pancreatic elastase (PPE) and subsequently the complex between I and HNE.
 IT 208113-53-5P 208113-55-7P 208113-57-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of peptidyl pentafluoroethyl ketones as inhibitors of human neutrophil elastase)
 RN 208113-53-5 CAPLUS
 CN 1-Pyrrolidineacetamide, 3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (3S)- (9CI) (CA INDEX NAME)

L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

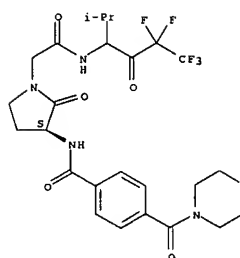


RN 244132-99-8 CAPLUS
 CN Butanoic acid, 3-[[[(2S)-2-[[[(3R)-3-[[2,6-dichlorobenzoyl]amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

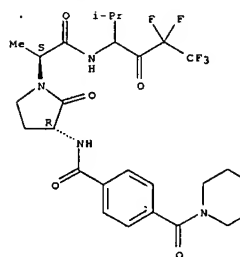


L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 Absolute stereochemistry.



RN 208113-55-7 CAPLUS
 CN 1-Pyrrolidineacetamide, alpha-methyl-3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (3S,3R)- (9CI) (CA INDEX NAME)

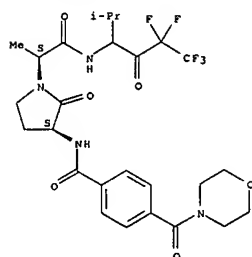
Absolute stereochemistry.



RN 208113-57-9 CAPLUS
 CN 1-Pyrrolidineacetamide, alpha-methyl-3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (3S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

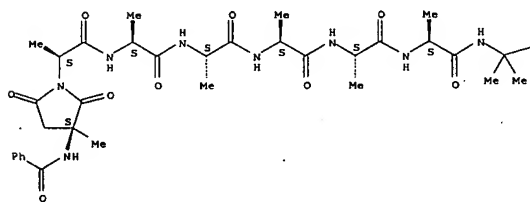
ACCESSION NUMBER: 1997:646051 CAPLUS
DOCUMENT NUMBER: 127:307651
TITLE: Design and synthesis of novel nonpolar host peptides for the determination of the 310- and α -helix compatibilities of α -amino acid building blocks: an assessment of α,α -disubstituted glycines
AUTHOR(S): Obrecht, Daniel; Altorfer, Michael; Bohdal, Udo; Daly, John; Huber, Walter; Labhardt, Alexander; Lehmann, Christian; Muller, Klaus; Ruffieux, Ruth; Schonholzer, Peter; Spiegler, Clive; Zumbrunn, Cornelia
CORPORATE SOURCE: F. Hoffmann-La Roche AG, Pharma Research, Basel, CH-4070, Switz.
SOURCE: Biopolymers (1997), 42(5), 575-626
CODEN: BIPMAJ; ISSN: 0006-3525
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present work describes three novel nonpolar host peptide sequences that provide a ready assessment of the 310- and α -helix compatibilities of natural and unnatural amino acids at different positions of small- to medium-size peptides. The unpolar peptides containing Ala, α -aminoisobutyric acid (Aib), and a C-terminal p-iodobenilide group were designed in such a way that the peptides could be rapidly assembled in a modular fashion, were highly soluble in solvent mixts. of trifluoroethanol and H₂O for CD and two-dimensional NMR analyses, and showed excellent crystallinity suited for x-ray structure anal. To validate this approach, 9-mer peptides, 12-mer peptides, and 10-mer peptides incorporating a series of optically pure cyclic and open-chain (R)- and (S)- α,α -disubstituted glycines were prepared. These amino acids are known to significantly modulate the conformations of small peptides. Based on x-ray structures, CD spectra recorded in acidic, neutral, and basic media and detailed 2D-NMR analyses, several interesting conformational observations were made. Especially interesting results were obtained using the convex constraint CD anal. proposed by Fasman, which allowed the determination of the relative content of 310- and α -helical conformations. These results were fully supported by the corresponding x-ray and 2D-NMR analyses. As a striking example, it was found that the (S)- and (R)- β -tetralin derived amino acids show excellent α -helix stabilization, more pronounced than Aib and Ala. These novel reference peptide sequences should help establish a scale for natural and unnatural amino acids concerning their intrinsic 310- and α -helix compatibilities at different positions of medium-sized peptides and thus improve the understanding of folding processes in peptides.
IT 197381-77-4P 197381-80-9P 197382-01-7P
197382-03-9P 197382-05-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (design and synthesis of novel nonpolar host peptides for determination of 310-

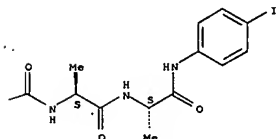
L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

and α -helix compatibilities of disubstituted glycine building blocks)
RN 197381-77-4 CAPLUS
CN L-Alaninamide, N-[(2S)-2-[(3S)-3-(benzoylamino)-3-methyl-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (-).

PAGE 1-A



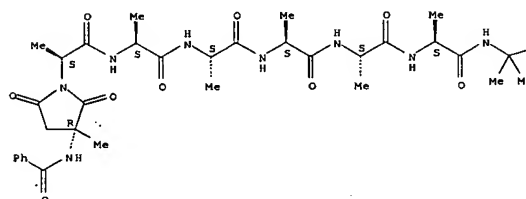
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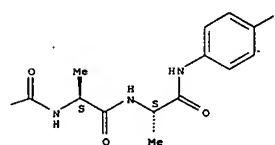
RN 197381-80-9 CAPLUS
CN L-Alaninamide, N-[(2S)-2-[(3R)-3-(benzoylamino)-3-methyl-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (+).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



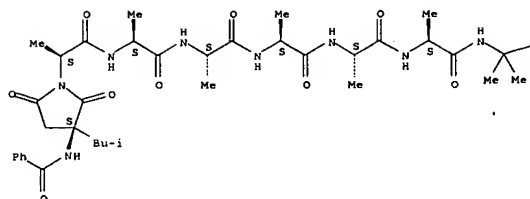
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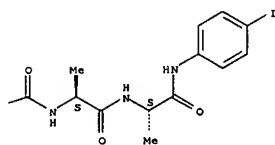
RN 197382-01-7 CAPLUS
CN L-Alaninamide, N-[(2S)-2-[(3S)-3-(benzoylamino)-3-(2-methylpropyl)-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)
Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

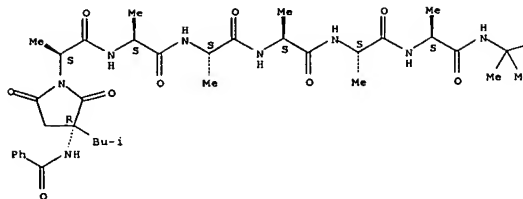


RN 197382-03-9 CAPLUS
 CN L-Alaninamide, N-[(2S)-2-[(3R)-3-(benzoylamino)-3-(2-methylpropyl)-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

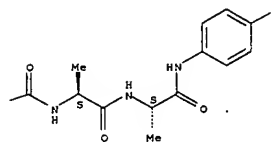
Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



RN 197382-05-1 CAPLUS
 CN L-Alaninamide, N-[(2S)-2-[(3S)-3-(benzoylamino)-3-methyl-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)-, compd. with acetonitrile (1:5) (9CI) (CA INDEX NAME)

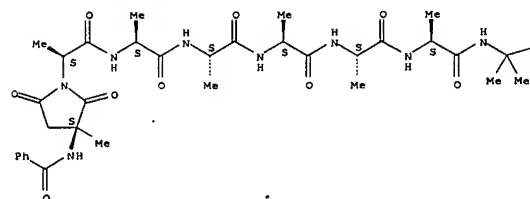
CM 1

CRN 197381-77-4
 CMF C46 H62 I N11 O12

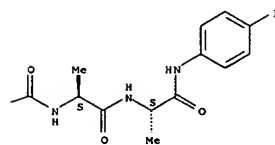
Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B



CM 2

CRN 75-05-8
 CMF C2 H3 N

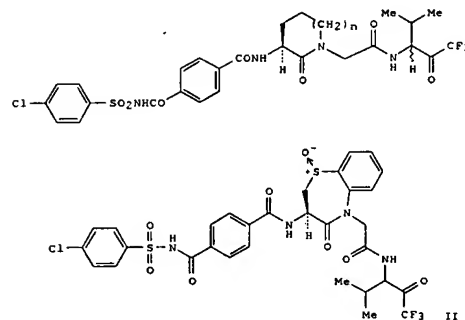
H₃C-C≡N

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L12 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:135101 CAPLUS
 DOCUMENT NUMBER: 120:135101
 TITLE: Elastase inhibitors containing conformationally restricted lactams as P3-P2 dipeptide replacements
 AUTHOR(S): Skiles, Jerry W.; Sorcek, Ronald; Jacober, Stephen; Miao, Clara; Mui, Philip W.; McNeil, Daniel; Rosenthal, Alan S.
 CORPORATE SOURCE: Dep. Med. Chem., Boehringer Ingelheim Pharm., Inc., Ridgefield, CT, 06877, USA
 SOURCE: Bioorganic & Medicinal Chemistry Letters (1993), 3(4),
 773-8
 CODEN: BMCLE8; ISSN: 0960-894X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 120:135101
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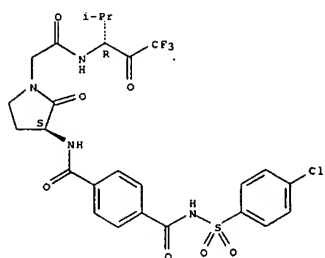


AB Title conformationally restricted lactams I (n = 0, 1, 2) and II were prepared as potential human leukocyte elastase (HLE) inhibitors.
 IT 152839-11-7P 152839-12-8P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as human leukocyte elastase inhibitor)
 RN 152839-11-7 CAPLUS
 CN 1,4-Benzenedicarboxamide,
 N-[(4-chlorophenyl)sulfonyl]-N'-(2-oxo-1-[2-oxo-2-[[3,3,3-trifluoro-1-(1-methylethyl)-2-oxopropyl]amino]ethyl]-3-pyrrolidinyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

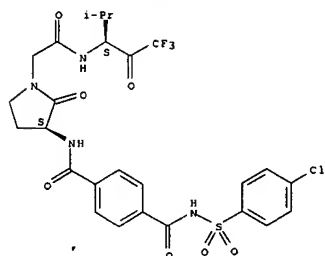
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L12 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 152839-12-8 CAPLUS
 CN 1,4-Benzenedicarboxamide,
 N-[(4-chlorophenyl)sulfonyl]-N'-[2-oxo-1-[2-oxo-
 2-[(3,3,3-trifluoro-1-[(1-methylethyl)-2-oxopropyl]amino]ethyl]-3-
 pyrrolidinyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:8140 CAPLUS
 DOCUMENT NUMBER: 50:8140
 ORIGINAL REFERENCE NO.: 50:1590h-1,1591a-h
 TITLE: Studies on specific chemical fission of peptide
 links.

AUTHOR(S): I. Rearrangements of aspartyl and glutamyl peptides
 Battersby, Alan R.; Robinson, J. C.
 CORPORATE SOURCE: Univ. St. Andrews, UK
 SOURCE: Journal of the Chemical Society (1955) 259-69
 CODEN: JCSQA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 49, 864f. The esters of α- and β-aspartyl peptides,
 RCONHCH(CH₂CO₂Et)CONHR' and RCONHCH(CO₂Et)CH₂CONHR', are converted by
 alkaline

hydrolysis into mixts. of aspartyl peptides, RCONHCH(CO₂H)CH₂CONHR' and
 RCONHCH(CH₂CO₂H)CONHR', the former product preponderating.
 DL-BzNHCH(CO₂H)CH₂CO₂Et (I), m. 105-7°, was prepared from β-Et
 DL-aspartate-HCl, K₂CO₃ and BzCl; and DL-BzNHCH(CO₂H)CH₂CH₂CO₂Et, m.
 114-15.5°, was prepared by benzylation of γ-Et DL-glutamate.
 A stirred solution of I and Et₃N (II) in dioxane and CHCl₃ was treated at
 0° with ClCO₂Et (III), an excess of NH₄OH added after 20 min., and
 the stirring continued for 5 hrs. After addition of water, the solution

was acidified and concentrated, yielding DL-BzNHCH(CH₂CO₂Et)CONH₂ (IV), m.
 151-3°. The reaction between NH₃ and N-benzoyl-DL-aspartic
 anhydride (V) yields DL-BzNHCH(CO₂H)CH₂CONH₂ (VI), m. 189-90° and a
 small amount of DL-BzNHCH(CH₂CO₂H)CONH₂ (VII), m. 208-9°. VI is also
 obtained from the reaction of I and dilute NH₃, or upon the racemization

of the L-amide. BzNHCH.CO.NH.CO.CH₂ (VIII), m. 223-5°, prepared by the
 reaction of NaOH or NaOEt with IV, forms DL-BzNHCH(CO₂H)CH₂CONH₂, m.
 270°, upon treatment with NH₄OH. DL-BzNHCH(CO₂Et)CH₂CO₂Et (IX), m.
 75-7°, was prepared by the reaction of the free acid with EtOH and
 dry HCl. Refluxing V with absolute EtOH yields IX, I, and
 DL-BzNHCH(CO₂Et)CH₂CO₂H, m. 111-12.5°. DL-BzNHCH(CO₂Et)CH₂CONH₂,
 m. 152-4°, was synthesized in a manner similar to IV. IV could not
 be cyclized by treatment with HBr in MeNO₂ or HCl in EtOH. The action of
 alkali on IV or VIII yields mainly VI and a small amount of VII.

n-C₆H₁₃NH₂ in dioxane was added to a solution of phthaloylglycyl chloride and the
 solution concentrated. Addition of 0.5% NaHCO₃ gave a precipitate of
 phthaloylglycine n-hexylamide,

m. 164-6°, which upon refluxing with H₂O followed by
 acidification gave Me(CH₂)₅NHCOCH₂CH₂CHCl (X), m. 249°. A solution of
 benzyloxycarbonylglycylglycine and II in CHCl₃ when treated at 0°
 with III followed by addition of γ-Et L-glutamate in 0.1N NaOH, yields
 PhCH₂COCONHCH₂CONHCH₂CONHCH(CO₂H)CH₂CH₂CO₂Et, m. 151-3°.
 Me(CH₂)₅NHCOCH₂CH₂NHCO₂Et, m. 94-5°, was prepared from III, X, and II.
 Glycine n-hexylamides of acylaspartic and -glutamic acid monoesters can

be prepared by the reaction of the monoester in dioxane-CHCl₃ with II and
 III

L12 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

at 0° followed by X. DL-BzNHCH(CH₂CO₂Et)CONHCH₂CONH(CH₂)₅Me (XI),
 m. 105-7°, DL-BzNHCH(CO₂Et)CH₂CONHCH₂CONH(CH₂)₅Me (XII), m.
 82-7°, DL-BzNHCH(CH₂CH₂CO₂Et)CONHCH₂CONH(CH₂)₅Me (XIII), m.
 110-12°, and 1-PhCH₂COCONHCH₂CONHCH₂CONHCH(CH₂CH₂CO₂Et)CONHCH₂CONH(CH₂)₅Me (XIV), m. 142-3°, [α]_D²⁰ 3.6°, were thus prepd.
 The reaction between X and II with V yields DL-
 BzNHCH(CH₂CO₂H)CONHCH₂CONH(CH₂)₅Me (XV), m. 179-80°, and
 DL-BzNHCH(CO₂H)CH₂CONHCH₂CONH(CH₂)₅Me (XVI), m. 163-4°. XV was
 also obtained by refluxing XI with HCl and Me₂CO. DL-
 BzNHCH(CH₂CONH₂)CONHCH₂CONH(CH₂)₅Me (XVII), m. 186-7°, was prepd.
 from XV in a manner similar to the prepn. of IV. XVII is also obtained

by treatment of XI with satd. alc. NH₃. A soln. of XIV and AcOH in MeOH was
 shaken with H and Pd until CO₂ evolution was complete. The filtered
 soln.

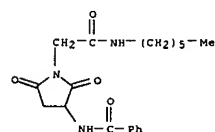
was evapd. to a gum, the unreacted XIV removed, and the rest shaken with
 Ac₂O. Evapn. gave a gum from which L-AcNHCH₂CONHCH₂CONHCH(CH₂CH₂CO₂Et)
 CONHCH₂CONH(CH₂)₅Me (XVIII), m. 193.5-4.5°, was isolated. XV, XVI
 and DL-benzamidosuccinoylglycine n-hexylamide, m. 149-50°, are
 obtained by the action of alkali on XI or XII, whereas
 BzNHCH(CO₂H)CH₂CH₂CONHCH₂CONH(CH₂)₅Me (XIX), m. 129-31°, and
 BzNHCH(CH₂CH₂CO₂H)CONHCH₂CONH(CH₂)₅Me (XX), m. 184-6°, are obtained
 from XIII. XVIII reacts with aq. NaOH to form L-
 AcNHCH₂CONHCH₂CONHCH(CH₂CH₂CO₂H)CONHCH₂CONH(CH₂)₅Me, m. 185-7°.
 XIX and XX were prepd. from X and N-benzoylglutamic anhydride, m.
 154-5°, by the method used for the aspartyl analogs. The possible
 application of the observed rearrangements in a scheme for the specific
 fission of a peptide chain at the aspartic and glutamic residues are
 discussed.

IT 857423-00-8P, 1-Pyrrolidineacetamide, 3-benzamido-N-hexyl-2,5-
 dioxo-

RL: PREP (Preparation)
 (preparation of)

RN 857423-00-8 CAPLUS

CN 1-Pyrrolidineacetamide, 3-benzamido-N-hexyl-2,5-dioxo- (5CI) (CA INDEX
 NAME)



=> log h

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	44.95	397.81
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CA SUBSCRIBER PRICE	-6.00	-6.00

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STN INTERNATIONAL SESSION SUSPENDED AT 10:33:26 ON 13 DEC 2006

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PASSWORD:

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SESSION RESUMED IN FILE 'MEDLINE, CAPLUS' AT 10:45:46 ON 13 DEC 2006
FILE 'MEDLINE' ENTERED AT 10:45:46 ON 13 DEC 2006
FILE 'CAPLUS' ENTERED AT 10:45:46 ON 13 DEC 2006
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	44.95	397.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-6.00	-6.00

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	44.95	397.81
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-6.00	-6.00

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STRUCTURE FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1
DICTIONARY FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

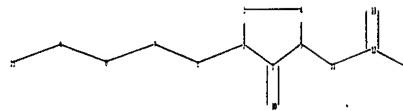
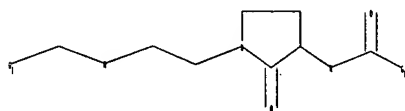
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=>

Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 4.str



chain nodes :

6 7 8 9 10 11 12 13 14 15

ring nodes :

1 2 3 4 5

chain bonds :

1-10 2-6 5-11 6-7 7-8 8-9 9-15 11-12 12-13 12-14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 5-11 7-8 8-9 9-15 11-12 12-13 12-14

exact bonds :

10776586.trn

6-7

G1:Cb,Cy,Hy

Match level :

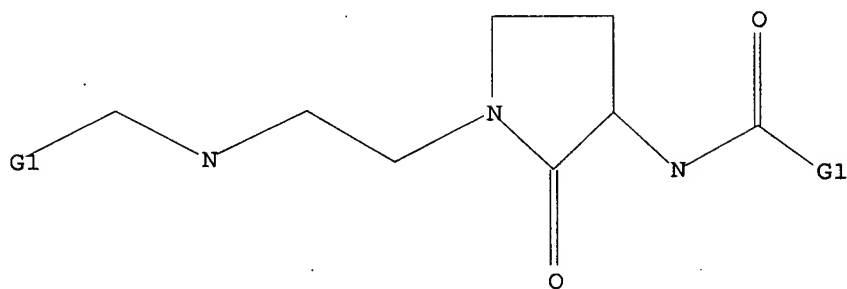
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10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L13 STRUCTURE UPLOADED

=> d

L13 HAS NO ANSWERS

L13 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> l13

SAMPLE SEARCH INITIATED 10:46:06 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 79 TO ITERATE

100.0% PROCESSED 79 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1047 TO 2113

PROJECTED ANSWERS: 1 TO 80

L14 1 SEA SSS SAM L13

=> l13 full

FULL SEARCH INITIATED 10:46:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1291 TO ITERATE

100.0% PROCESSED 1291 ITERATIONS

32 ANSWERS

SEARCH TIME: 00.00.01

L15 32 SEA SSS FUL L13

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	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-6.00

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FILE 'CAPLUS' ENTERED AT 10:46:20 ON 13 DEC 2006
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=> l15
 L16 3 L15

=> d his

(FILE 'HOME' ENTERED AT 10:26:24 ON 13 DEC 2006)

FILE 'REGISTRY' ENTERED AT 10:26:36 ON 13 DEC 2006

L1 STRUCTURE UPLOADED
 L2 50 L1
 L3 STRUCTURE UPLOADED
 L4 50 L3
 L5 874 L3 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:27:48 ON 13 DEC 2006

L6 300 L5
 L7 284 DUP REM L6 (16 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006

L8 STRUCTURE UPLOADED
 L9 1 L8
 L10 23 L8 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:28:52 ON 13 DEC 2006

L11 8 L10
 L12 8 DUP REM L11 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 10:45:52 ON 13 DEC 2006

L13 STRUCTURE UPLOADED
 L14 1 L13
 L15 32 L13 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:46:20 ON 13 DEC 2006

L16 3 L15

=> l15 not l12
 L17 2 L15 NOT L12

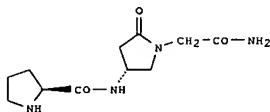
=> l16 not l12
 L18 2 L16 NOT L12

Page 20

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L18 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:645705 CAPLUS
 DOCUMENT NUMBER: 140:87048
 TITLE: iso-Lactam and reduced amide analogues of the peptidomimetic dopamine receptor modulator 3(R)-[2(S)-pyrrolidinylcarbonyl]amino]-2-oxo-1-pyrrolidineacetamide
 AUTHOR(S): Dolbeare, Kristine; Pontoriero, Giuseppe F.; Gupta, Suresh K.; Mishra, Ram K.; Johnson, Rodney L.
 CORPORATE SOURCE: Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
 SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(18), 4103-4112
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:87048
 GI



I

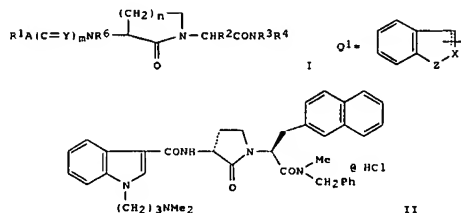
AB 4(R)-[[2(S)-pyrrolidinylcarbonyl]amino]-2-oxo-1-pyrrolidineacetamide (I), an analog of the title γ -lactam Pro-Leu-Gly-NH₂ peptidomimetic and a series of other analogs were synthesized. The compds. were tested for their ability to enhance the binding of [³H]N-propylnorapomorphine to dopamine receptors in a functional in vitro assay utilizing bovine striatal membranes.
 IT 644996-25-8P
 RL: BVP (Byproduct); PREP (Preparation)
 (preparation of pyrrolidineacetamides as peptidomimetic dopamine receptor modulators)
 RN 644996-25-8 CAPLUS
 CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3R)-2-oxo-1-[[[(2S)-1-[(phenylmethoxy)carbonyl]-2-pyrrolidinyl]carbonyl]amino]ethyl]-3-pyrrolidinyl]amino]carbonyl]-, phenylmethyl ester, (2S)- (9CI) (CA INDEX NAME)
 Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:135143 CAPLUS
 DOCUMENT NUMBER: 120:135143
 TITLE: Preparation of peptides with tachykinin antagonist activity
 INVENTOR(S): Matsuo, Masaaki; Hagiwara, Daijiro; Miyake, Hiroshi; Igarashi, Norihito; Murano, Kenji
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 73 pp.
 CODEN: PIXX2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

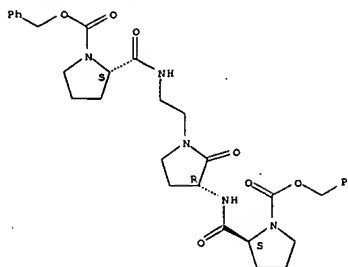
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9314113	A1	19930722	WO 1993-JP2	19930104
W: CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 620824	A1	19941026	EP 1993-900452	19930104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07503711	T2	19950420	JP 1993-512326	19930104
PRIORITY APPLN. INFO.:			GB 1992-535	A 19920110
			WO 1993-JP2	W 19930104

OTHER SOURCE(S): MARPAT 120:135143
 GI



AB Title compds. (I: R1 = (substituted) aryl, pyridyl, pyrrolyl, Q1: dotted line = optional double bond; X = CH, N; Z = O, S, NH; R2, R4 = (substituted) aralkyl; R3 = (substituted) alkyl; R6 = H, alkyl; A = bond, alkylene, alkenylene; Y = O, NR7; R7 = H, alkyl; m = 0, 1; n = 0, 2).
 were prepared Thus, title compound II, prepared by solution phase methods, at 10 mg/kg orally in guinea pigs gave 95.7% inhibition of substance P-induced bronchoedema.
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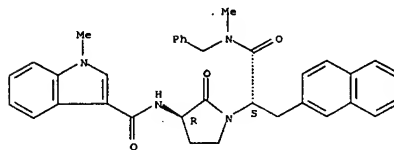
L18 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

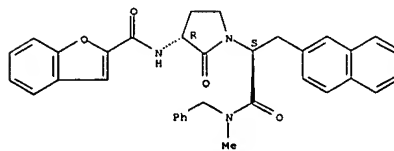
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 153050-31-8P 153050-32-9P 153050-33-0P
 153050-34-1P 153050-35-2P 153050-36-3P
 153050-37-4P 153050-38-5P 153050-40-9P
 153050-41-0P 153050-42-1P 153050-43-2P
 153050-44-3P 153050-45-4P 153050-46-5P
 153050-47-6P 153050-48-7P 153050-50-1P
 153050-51-2P 153050-52-3P 153050-53-4P
 153050-55-6P 153050-56-7P 153090-78-9P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of, as tachykinin antagonist)
 RN, 153050-31-8 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-methyl-N-[1-(2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl)-, [S-(R*,S*)]- (9CI)
 (CA INDEX NAME)
 Absolute stereochemistry.



RN 153050-32-9 CAPLUS
 CN 1-Pyrrolidineacetamide, 3-[[2-benzofuranylcarbonyl]amino]-N-methyl-N-[(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

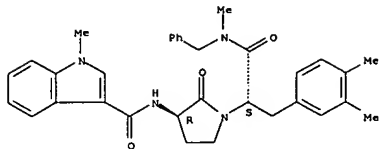
Absolute stereochemistry.



RN 153050-33-0 CAPLUS
 CN 1H-Indole-3-carboxamide, N-[1-[(3,4-dimethylphenyl)methyl]-2-[methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-1-methyl-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

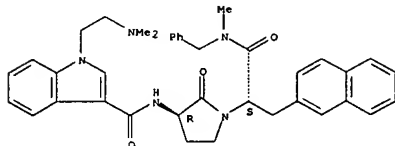
Absolute stereochemistry.



RN 153050-34-1 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-35-2 CAPLUS

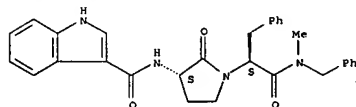
CN Carbamic acid, [2-[3-[[[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-1H-indol-1-yl]ethyl]-, 1,1-dimethylethyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CN 1H-Indole-3-carboxamide, N-[1-[2-(methyl(phenylmethyl)amino)-2-oxo-1-(phenylmethyl)ethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

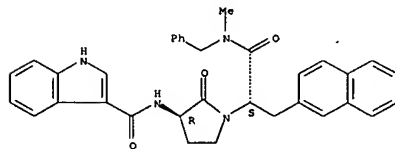
Absolute stereochemistry.



RN 153050-40-9 CAPLUS

CN 1H-Indole-3-carboxamide, N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

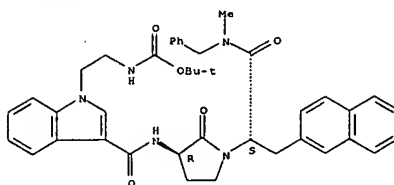


RN 153050-41-0 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

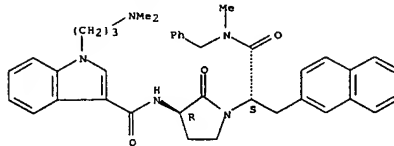
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 153050-36-3 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

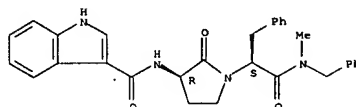
Absolute stereochemistry.



RN 153050-37-4 CAPLUS

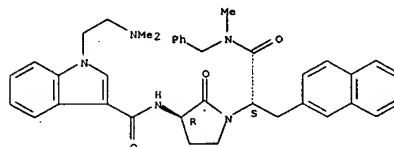
CN 1H-Indole-3-carboxamide, N-[1-[2-(methyl(phenylmethyl)amino)-2-oxo-1-(phenylmethyl)ethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-38-5 CAPLUS

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

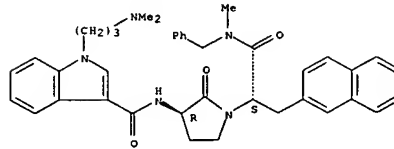


● HCl

RN 153050-42-1 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



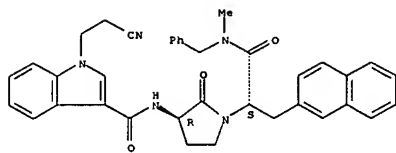
● HCl

RN 153050-43-2 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[2-(cyanoethyl)-N-[1-[2-(methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

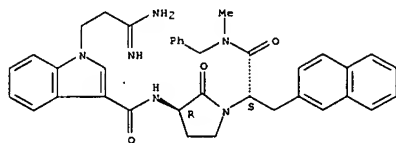
Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 153050-44-3 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(3-amino-3-iminopropyl)-3-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

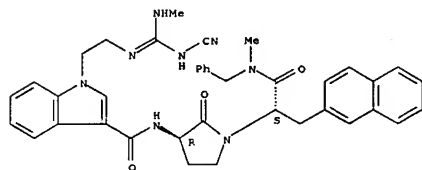


● HCl

RN 153050-45-4 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(2-aminoethyl)-N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

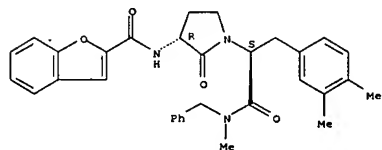
Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



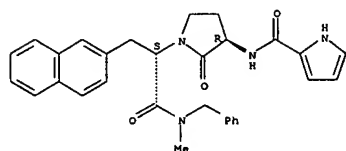
RN 153050-48-7 CAPLUS
 CN 1-Pyrrolidineacetamide, 3-[[[(2-benzofuran-2-ylcarbonyl)amino]-N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-50-1 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

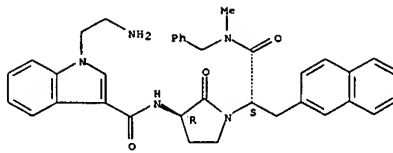
Absolute stereochemistry.



RN 153050-51-2 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(2-(dimethylamino)ethyl)-N-methyl-N-[[1-[(3,4-dimethylphenyl)methyl]-2-methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

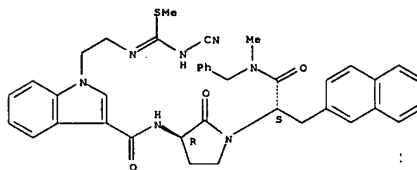
10776586.trn

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HCl

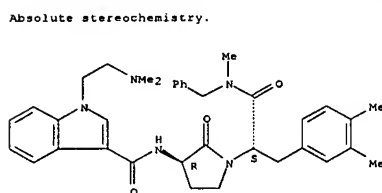
RN 153050-46-5 CAPLUS
 CN Carbamimidethioic acid, N-cyano-N'-[2-[3-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-1H-indol-1-yl]ethyl]-, methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 153050-47-6 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(2-[[[(cyanamino)(methylamino)methylene]amino]ethyl)-N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

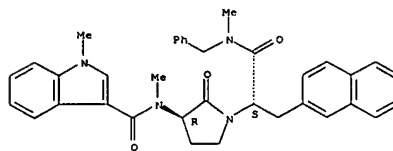
Absolute stereochemistry.
Double bond geometry unknown.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



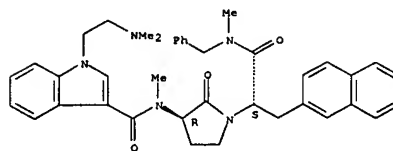
RN 153050-52-3 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(2-[[[(cyanamino)(methylamino)methylene]amino]ethyl)-N-methyl-N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-53-4 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[(2-[[[(cyanamino)(methylamino)methylene]amino]ethyl)-N-methyl-N-[[1-[(2-methyl(phenylmethyl)amino)-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

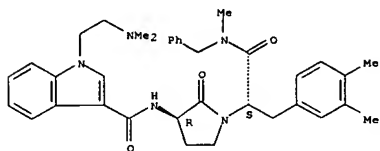
Absolute stereochemistry.



RN 153050-55-6 CAPLUS

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[1-[(3,4-dimethylphenyl)methyl]-2-[methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

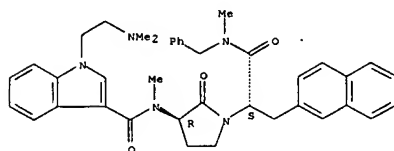
Absolute stereochemistry.



● HCl

RN 153050-56-7 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-methyl-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

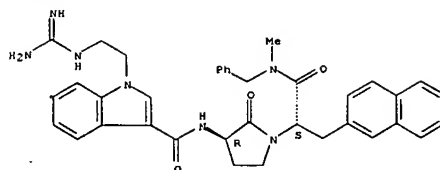


● HCl

RN 153090-78-9 CAPLUS
 CN 1H-Indole-3-carboxamide, 1-[2-[(aminoiminomethyl)amino]ethyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

15.36

580.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.50

-7.50

FILE 'REGISTRY' ENTERED AT 10:51:21 ON 13 DEC 2006

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

DICTIONARY FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

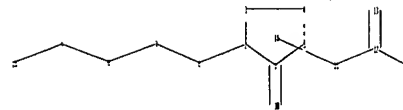
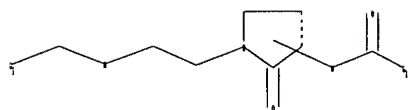
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 5.str



chain nodes :

6 7 8 9 10 11 12 13 14 15

ring nodes :

1 2 3 4 5

chain bonds :

1-10 2-6 6-7 7-8 8-9 9-15 11-12 12-13 12-14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9 9-15 11-12 12-13 12-14

exact bonds :

6-7

G1:Cb,Cy,Hy

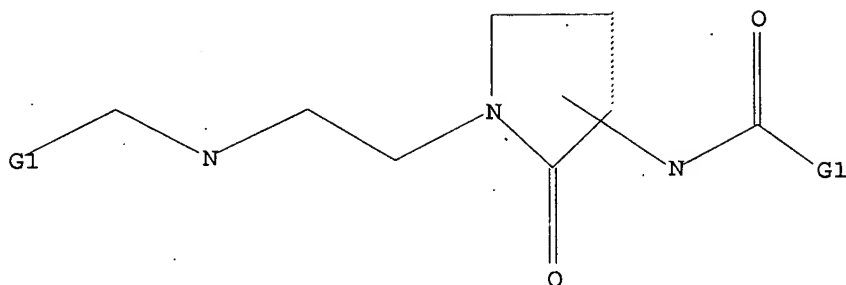
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS

L19 STRUCTURE UPLOADED

10776586.trn

=> d
L19 HAS NO ANSWERS
L19 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> l19
SAMPLE SEARCH INITIATED 10:51:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2466 TO ITERATE

81.1% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 46342 TO 52298
PROJECTED ANSWERS: 0 TO 0

L20 0 SEA SSS SAM L19

=> l19 full
FULL SEARCH INITIATED 10:51:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 49992 TO ITERATE

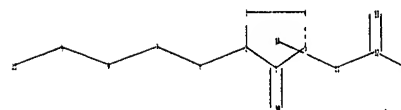
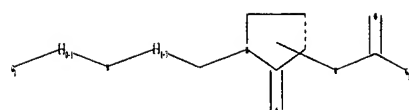
100.0% PROCESSED 49992 ITERATIONS
SEARCH TIME: 00.00.01

32 ANSWERS

L21 32 SEA SSS FUL L19

=> l21 not l15
L22 0 L21 NOT L15

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 6.str



chain nodes :

6 7 8 9 10 11 12 13 14 15

ring nodes :

1 2 3 4 5

chain bonds :

1-10 2-6 6-7 7-8 8-9 9-15 11-12 12-13 12-14

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9 9-15 11-12 12-13 12-14

exact bonds :

6-7

G1:Cb,Cy,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS

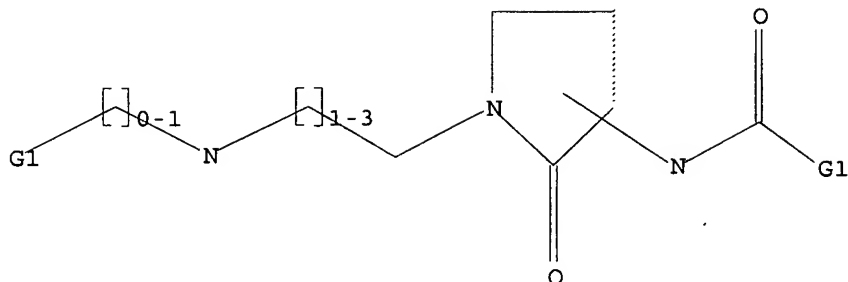
L23 STRUCTURE UPLOADED

10776586.trn

=> d

L23 HAS NO ANSWERS

L23 STR



G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> l23

SAMPLE SEARCH INITIATED 10:53:56 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 5114 TO ITERATE

39.1% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 97992 TO 106568
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

=> l23 full

FULL SEARCH INITIATED 10:54:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 104500 TO ITERATE

100.0% PROCESSED 104500 ITERATIONS
SEARCH TIME: 00.00.04

42 ANSWERS

L25 42 SEA SSS FUL L23

=> file medline caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
335.20	915.31

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-7.50

CA SUBSCRIBER PRICE

FILE 'MEDLINE' ENTERED AT 10:54:14 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:54:14 ON 13 DEC 2006

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=> l25

L26 5 L25

=> d his

(FILE 'HOME' ENTERED AT 10:26:24 ON 13 DEC 2006)

FILE 'REGISTRY' ENTERED AT 10:26:36 ON 13 DEC 2006

L1 STRUCTURE UPLOADED

L2 50 L1

L3 STRUCTURE UPLOADED

L4 50 L3

L5 874 L3 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:27:48 ON 13 DEC 2006

L6 300 L5

L7 284 DUP REM L6 (16 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006

L8 STRUCTURE UPLOADED

L9 1 L8

L10 23 L8 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:28:52 ON 13 DEC 2006

L11 8 L10

L12 8 DUP REM L11 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 10:45:52 ON 13 DEC 2006

L13 STRUCTURE UPLOADED

L14 1 L13

L15 32 L13 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:46:20 ON 13 DEC 2006

L16 3 L15

L17 2 L15 NOT L12

L18 2 L16 NOT L12

FILE 'REGISTRY' ENTERED AT 10:51:21 ON 13 DEC 2006

L19 STRUCTURE UPLOADED

L20 0 L19

L21 32 L19 FULL

L22 0 L21 NOT L15

L23 STRUCTURE UPLOADED

L24 0 L23

L25 42 L23 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 10:54:14 ON 13 DEC 2006

L26 5 L25

=> l26 not l12

L27 4 L26 NOT L12

=> l27 not l18

Page 31

L28 2 L27 NOT L18

=> d ibib abs hitstr 1-2

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:516307 CAPLUS

DOCUMENT NUMBER: 125:276500

TITLE: Synthesis, conformational properties, and synthetic applications of novel optically pure α,α -disubstituted (R)- and (S)-glycines (α chimeras) combining side chains of Asp, Glu, Leu, Phe, Ser, and Val

AUTHOR(S): Obrecht, Daniel; Abrecht, Christine; Altorfer, Michael; Bohdal, Udo; Grieder, Alfred; Kleber, Martina; Pflyffer, Patrick; Mueller, Klaus

CORPORATE SOURCE: Hoffmann-La Roche A.-G., Basel, CH-4002, Switz.

SOURCE: Helvetica Chimica Acta (1996), 79(5), 1315-1337

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of novel open-chain and cyclic conformationally constrained α,α -disubstituted (R)- and (S)-glycine deriva. (α -chimeras) combining side chains of Asp, Glu, Leu, Phe, Ser, and Val were efficiently prepared by α -alkylation of racemic 4-monosubstituted 2-phenyl-1,3-oxazol-5(4H)-ones, resolution after reaction with (S)-phenylalanine cyclohexylamide as chiral auxiliary, a novel azolactone/dihydrooxazole interconversion reaction to synthesize optically pure α -substituted (R) and (S)-serine deriva. coupled with succinimide-ring formation of aspartic acid deriva. Based on X-ray structures, the absolute configuration of these novel amino-acid building blocks was unambiguously determined and their preferred conformations in the crystalline state were assessed.

IT 182176-33-6P 182268-07-1P

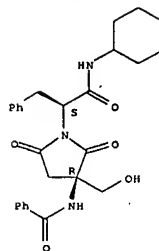
RI: PKP (Properties); SPN (Synthetic preparation); PREP (Preparation) (CD spectra; synthesis, conformation, and synthetic applications of α,α -disubstituted glycines)

RN 182176-33-6 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(hydroxymethyl)-2,5-dioxo-u-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

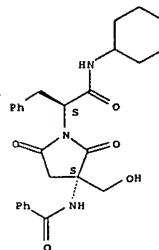
L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 182268-07-1 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(hydroxymethyl)-2,5-dioxo-u-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 182176-31-4P 182176-36-9P 182268-06-0P

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis, conformation, and synthetic applications of α,α -disubstituted glycines)

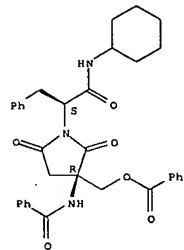
RN 182176-31-4 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-3-[(benzoyloxy)methyl]-N-

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

cyclohexyl-2,5-dioxo-u-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

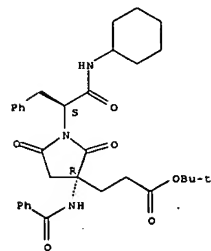
Absolute stereochemistry.



RN 182176-36-9 CAPLUS

CN 3-Pyrrolidinepropanoic acid, 3-(benzoylamino)-1-[2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-2,5-dioxo-, 1,1-dimethylethyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



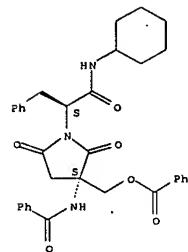
RN 182268-06-0 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-3-[(benzoyloxy)methyl]-N-cyclohexyl-2,5-dioxo-u-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10776586.trn

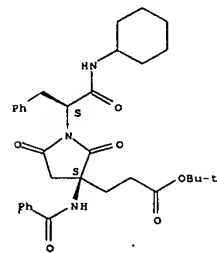
L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 182268-08-2 CAPLUS

CN 3-Pyrrolidinepropanoic acid, 3-(benzoylamino)-1-[2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-2,5-dioxo-, 1,1-dimethylethyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:842202 CAPLUS

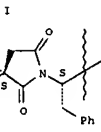
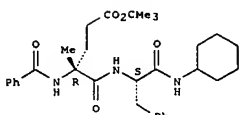
DOCUMENT NUMBER: 124:56605

TITLE: A novel synthesis of (R)- and (S)- α -alkylated aspartic and glutamic acids: α -alkylated aspartic succinimides as new type of β -turn type II and II' mimetics

AUTHOR(S): Obrecht, Daniel; Bohdel, Udo; Daly, John; Lehmann, Christian; Schoenholzer, Peter; Mueller, Klaus
 CORPORATE SOURCE: Pharma Res., F. Hoffmann-La Roche AG, Basel, CH-4002, Switz.

SOURCE: Tetrahedron (1995), 51(40), 10883-900
 CODEN: TETRAE; ISSN: 0040-4020

PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:56605
 GI



AB A novel and efficient synthesis of optically pure (R)- and (S)- α -methylglutamic acid, (R)- and (S)- α -methylaspartic acid, and (R)- and (S)- α -isobutylaspartic acid, using L-phenylalanine cyclohexylamide as chiral auxiliary, is described. Crystal structures show that the (R)- (I) (R,S-configuration) and (S)- α -methylglutamic acid derivs. adopt β -turn type I geometries, whereas the corresponding aspartimide derivs. II (R = Me, isobutyl) (R,S) form a β -turn type II and III (S,S) a β -turn type II'. These findings suggest that the succinimide derivs. of (R)- and (S)- α -alkylaspartic acids can serve as building blocks to stabilize β -turns of type II (or II') in peptides, depending on their absolute configuration.

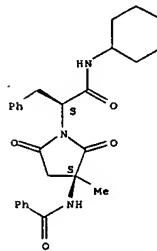
IT 172095-19-1P 172275-38-6P 172275-39-7P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis and conformation of alkylated aspartic and glutamic acids and aspartic succinimide derivs.)

L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 172095-19-1 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-methyl-2,5-dioxo- α -(phenylmethyl)-, [5-(R*,R*)]- (9CI) (CA INDEX NAME)

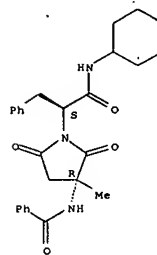
Absolute stereochemistry.



RN 172275-38-6 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-methyl-2,5-dioxo- α -(phenylmethyl)-, [5-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



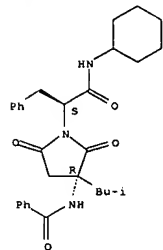
RN 172275-39-7 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(2-methylpropyl)-2,5-dioxo- α -(phenylmethyl)-, [5-(R*,S*)]- (9CI) (CA INDEX NAME)

L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

Absolute stereochemistry.



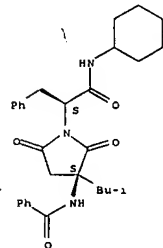
IT 172095-20-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis and conformation of alkylated aspartic and glutamic acids and aspartic succinimide derivs.)

RN 172095-20-4 CAPLUS

CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(2-methylpropyl)-2,5-dioxo- α -(phenylmethyl)-, [5-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> log h

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
11.91	927.22

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.50	-9.00

CA SUBSCRIBER PRICE

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:55:15 ON 13 DEC 2006